Isophthalic acid, monoamide, N-(2-bromophenyl)-, ethyl ester

Inchi: InChI=1S/C16H14BrNO3/c1-2-21-16(20)12-7-5-6-11(10-12)15(19)18-14-9-4-3-8-13(14)1

InchiKey: HNAQDMRCRNJUKF-UHFFFAOYSA-N

Formula: C16H14BrNO3

SMILES: CCOC(=O)c1cccc(C(O)=Nc2ccccc2Br)c1

Mol. weight [g/mol]: 348.19

Physical Properties

Property code	Value	Unit	Source
hf	-221.72	kJ/mol	Joback Method
hvap	92.75	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.262		Crippen Method
mcvol	225.270	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	939.99	K	Joback Method
tc	1182.22	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345793&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature